RADCALC—READ ME FIRST
RADCALC 4.0

CAUTION: *The following provides important information regarding the functionality and limitations of Radcalc 4.0. Use of Radcalc 4.0 implies you have read this file and understand it, and that you accept the disclaimer and distribution provisions in Section 1.5.*

1.0 INSTALLATION INSTRUCTIONS

1.1 SYSTEM REQUIRMENTS

Before installing Radcalc 4.0, you should make sure that your computer system meets (or exceeds) the following specifications:

1. PC-compatible computer.

2. Pentium processor, equivalent, or higher.

3. Microsoft[1] Windows[2] 98, NT[3] 4.0 or newer version of either operating system.

4. 32 megabyte of available space.

5. A printer driver must be installed on the operating system.

6. Internet Explorer[4] 6.0, Service Pack 1 or later version installed. This software may be downloaded free of charge from http://www.microsoft.com (Internet Explorer 6).

7. Microsoft Jet[5] 4.0, Service Pack 8 database engine installed. This software may be downloaded free of charge from http://www.microsoft.com (Microsoft Jet 4.0).

8. Microsoft Data Access Components (MDAC[6]), version 2.7, or newer installed (requires Administrative rights for installation). This software may be downloaded free of charge from http://www.microsoft.com (MDAC 2.8).

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[1] Microsoft is a registered trademark of the Microsoft Corporation, Redmond, Washington.
[2] Windows is a registered trademark of the Microsoft Corporation, Redmond, Washington.
[3] NT is a registered trademark of the Microsoft Corporation, Redmond, Washington.
[4] Explorer is a registered trademark of the Microsoft Corporation, Redmond, Washington.
[5] Jet is a registered trademark of the Microsoft Corporation, Redmond, Washington.
[6] MDAC is a registered trademark of the Microsoft Corporation, Redmond, Washington.

9. Microsoft .NET[7] redistributable framework, version 1.1 or newer installed (requires Administrative rights for installation). This software may be downloaded free of charge from http://www.microsoft.com (Microsoft .NET Framework Version 1.1 Redistributable).

10. In some cases it may be necessary to uninstall previous versions of the Radcalc software.

1.2 PREPARING COMPUTER FOR RADCALC 4.0

Radcalc uses several components from Microsoft that cannot be installed by the Radcalc setup program. Therefore, there are steps that the user must accomplish to prepare a computer to run Radcalc. Please perform the steps below in the sequence given.

1.2.1 Windows 3.1 and Windows 95

Radcalc is unable to operate on Windows 3.1 or Windows 95 systems.

1.2.2 Windows 98SE and Windows NT 4.0, Service Pack 6A

1. If not already installed, download Internet Explorer version 6.0 or later from the Microsoft website and install. Internet Explorer 6.1 is available from the Radcalc setup download. You can determine the version of Internet Explorer on your computer by launching Internet Explorer, clicking on "Help," and then clicking on "About Internet Explorer."

2. If not already installed, download the Microsoft Jet database engine version 4.0 from the Microsoft website and install. Microsoft Jet 4.0 is available from the Radcalc setup download. If you are not sure whether Microsoft Jet 4.0 or later is installed, it is safe to install it again.

3. If not already installed, download Windows Management Instrumentation (WMI[8]) Core version 1.5 or later. This software may be downloaded free of charge from http://www.microsoft.com (WMI Core 1.5).

4. If not already installed, download Microsoft Data Access Components (MDAC) version 2.7 or later from the Microsoft website and install. MDAC 2.8 is available from the Radcalc setup download. If you are not sure whether MDAC 2.7 or later is installed, it is safe to install it again.

5. If not already installed, download the .NET framework version 1.1 or later from the Microsoft website and install. The .NET framework 1.1 is available from the Radcalc setup download. If you are not sure whether .NET framework 1.1 or later is installed, it is safe to install it again.

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[7] .NET is a registered trademark of the Microsoft Corporation, Redmond, Washington.
[8] WMI is a registered trademark of the Microsoft Corporation, Redmond, Washington.

6. Install a printer driver on your computer, even if there is no printer attached to your computer. Radcalc does not care what printer driver you select, only that you have at least one installed.

1.2.3 Windows 2000 Service Pack 3 (or later) and Windows XP

1. Ensure the Windows 2000 is current to Service Pack 3 or later.

2. If not already installed, download Internet Explorer version 6.0 or later from the Microsoft website and install. Internet Explorer 6.1 is available from the Radcalc setup download. You can determine the version of Internet Explorer on your computer by launching Internet Explorer, clicking on "Help," and then clicking on "About Internet Explorer."

3. If not already installed, download Microsoft Data Access Components (MDAC) version 2.7 or later from the Microsoft website and install. MDAC 2.8 is available from the Radcalc setup download. If you are not sure whether MDAC 2.7 or later is installed, it is safe to install it again.

4. If not already installed, download the .NET framework version 1.1 or later from the Microsoft website and install. The .NET framework 1.1 is available from the Radcalc setup download. If you are not sure whether .NET framework 1.1 or later is installed, it is safe to install it again.

5. Install a printer driver on your computer, even if there is no printer attached to your computer. Radcalc does not care what printer driver you select, only that you have at least one installed.

1.3 DOWNLOADING AND INSTALLING RADCALC 4.0

1. Turn on your computer and enter the Windows environment.

2. Close all applications.

3. Connect to the Internet. In your web page browser type in http://www.doe-radcalc.com.

4. Logon, or register if you are a new user. New users will be E-mailed a password.

5. Select the Radcalc link.

6. When prompt appears select "save this file to disk"

7. Select the directory to install the zip file to. The default is your desktop.

8. When download is complete, select the zip file from Windows Explorer[9].

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[9] Explorer is a registered trademark of the Microsoft Corporation, Redmond, Washington.

9. Select "next" when winzip wizard appears.

10. The SETUP program will unzip the files in the directory of your choice. The default directory is C:\Program Files\Duratek\Radcalc 4.0.

11. Select "unzip".

12. Select "close" in the wizard window.

13. If the disk does not auto run, double click the Radcalc 4.0 setup file "setup.exe" to initiate installation.

1.4 INSTALLATION VERIFICATION

After Radcalc has been installed, it is recommended that the user validate correct installation. Start the Radcalc program. Once the program is running, go to the Tools menu in the menu bar at the top of the active Radcalc window and select "Tools" and then select "Validate Radcalc Installation." The software automatically runs a case and compares it to memory.

If the program is correctly installed it will display a report stating that proper validation was performed. Validating Radcalc before performing calculations is essential to ensure correct installation. A copy of the validation comparison file (VnVTest.rad) is located in the C:\Program Files\Duratek\Radcalc 4.0\Verify folder.

1.5 PATENT CAUTION

Radcalc may contain patentable subject matter protected from unauthorized disclosure under U.S. Patent Law (35 USC 205). No further dissemination is permitted outside of the government without the approval of the Assistant General Counsel for Intellectual Property, U.S. Department of Energy (DOE).

> **LEGAL DISCLAIMER**. This report was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor any agency thereof, nor any of their employees, nor any of their contractors, subcontractors or their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or any third party's use or the results of such use of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise, does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof or its contractors or subcontractors.   The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof or its contractors or subcontractors.

SOFTWARE DISTRIBUTION: This computer software has been developed under sponsorship of the DOE. Any further distribution or use by anyone other than the named licensee of the software package or any data contained therein, unless otherwise specifically provided for, is prohibited without the approval of the Energy Science and Technology Software Center. Requests for DOE-developed computer software shall be directed to the Energy Science and Technology Software Center, P.O. Box 1020, Oak Ridge, TN 37831-1020.

2.0 RADCALC CAPABILITIES

Radcalc is a user-friendly software application that may be used to automate packaging and transportation determinations for shipment of radioactive materials. Radcalc is used throughout the DOE Complex; by multiple federal, state, and international agencies; and by public and commercial organizations. Radcalc capabilities include the following.

- Performs transportation classification determinations based on selected U.S. Department of Transportation (DOT) definitions and methodologies outlined in 49 CFR, Subchapter C.

- Performs determinations or calculations in accordance with selected methods proscribed by the DOE, U.S. Nuclear Regulatory Commission (NRC), U.S. Environmental Protection Agency, and International Conference of Radiological Protection (ICRP).

- Calculates the decay heat and activity of radionuclides and their daughter products at a future date using a radioactive decay algorithm.

- Calculates the radiolytic production of hydrogen gas in a radioactive waste matrix.

2.1 DOT DETERMINATIONS

Radcalc provides the following DOT determinations for radioactive material shipments.

- Radioactive
- Type A or Type B
- Effective A_1 or A_2 for mixture
- Limited quantity
- Low specific activity, (LSA)-I, LSA-II, or LSA-III
- Highway route controlled quantity

- Fissile quantity
- Fissile excepted
- Reportable quantity.

Radcalc also provides a list of isotopes that are required for shipping papers and labels (95% of the total A_1/A_2 values). Radcalc has a transportation library including all isotopes identified in 49 CFR 173, "Shippers—General Requirements for Shipments and Packagings," 173.435, "Table of A_1 and A_2 values for radionuclides." DFSNW-ECAL-027, *Radcalc Regulatory Database* documents previously established regulatory values, which were consolidated in DFSNW-ECAL-030, *Radcalc Unified Database*. DTS-ECAL-259, *Radcalc 4.0 Unified Database* documents the updated regulatory values.

2.2 DOE DETERMINATIONS

Radcalc qualifies waste in accordance with selected DOE requirements including the following.

- Transuranic (TRU) waste classification in accordance with the DOE Manual M435.1-1, Chg. 1, *Radioactive Waste Management Manual.*

- ^{239}Pu-equivalent activity in accordance with DOE/WIPP-02-3122, *Contact-Handled Transuranic Waste Acceptance Criteria for the Waste Isolation Pilot Plant*, Rev. 1.

- ^{239}Pu fissile gram equivalent (FGE) calculations in accordance with the *TRUPACT-II Approved Methods for Payload Control (TRAMPAC)*, Rev. 19C (WTS 2003).

DFSNW-ECAL-030 documents previously established regulatory values, including those for DOE classifications; there have been no changes from the previously established DOE values.

2.3 NRC DETERMINATIONS

Radcalc categorizes radioactive contents in three levels of safety (Category I, II, or III) in accordance with NRC Regulatory Guide 7.11, *Fracture Toughness Criteria of Base Material for Ferritic Steel Shipping Cask Containment Vessels With a Maximum Wall Thickness of 4 inches (0.1 m)*. DFSNW-ECAL-030 documents previously established regulatory values, including those for NRC classifications; there have been no changes from the previously established NRC values.

2.4 DOSE-EQUIVALENT CURIE DETERMINATIONS

Radcalc capabilities have been expanded to calculate dose-equivalent curie (DE-Ci) values in accordance with FGR11/EPA-520/1-88-020, *Limiting Values of Radionuclide Intake and Air Concentration and Dose Conversion Factors for Inhalation, Submersion, and Ingestion*. In addition Radcalc capabilities have been expanded to calculate DE-Ci values in accordance with

ICRP 71, *Age-Dependent Doses to Members of the Public from Intake of Radionuclides: Part 4 Inhalation Dose* Coefficients, and ICRP 72, *Age-Dependent Doses to Members of the Public from Intake of Radionuclides: Part 5 Compilation of Ingestion and Inhalation Dose Coefficients*. DTS-ECAL-259, *Radcalc 4.0 Unified Database* documents the DE-Ci database values. Radcalc also has the capability to write .iso files for use with the DE-Calc software (previously referred to as Hazclass), DFSNW-VV-020, *Hazclass 1.0 Verification and Validation Test Report*, which calculates DE-Ci values for Hanford Site shipments.

2.5 RADIOACTVE DECAY DETERMINATIONS

Radcalc uses a decay data library containing 1,867 isotopes to calculate the activity of an isotope and its decay products over a specified period of time. Radcalc also calculates the decay heat of the nuclear material in the package. The Radcalc nuclear database is based on a combination of the *Fusion Evaluated Nuclear Data Library (FENDL)* (IAEA 1988) and the *Joint Evaluated File (JEF)* (OECD 1993). The Radcalc atomic mass database is based on "The NUBASE Evaluation of Nuclear and Decay Properties" (Audi 1997). The nuclear database is documented in WMTS-ECAL-028, *Radcalc Nuclear Database*, and the atomic mass database is documented in DFSNW-ECAL-029, *Radcalc Atomic Mass Database*; copies of these documents are provided in DFSNW-RPT-42, *Radcalc 3.0 Volume IV: Database Manual*. DFSNW-ECAL-030 consolidates these databases; there have been no changes from these previously established databases.

Users may input source term in grams, Becquerels or curies and convert between units; multiply the source term by a factor to increase or decrease activity; and import data from or export data to other Radcalc files or spreadsheet files.

2.6 HYDROGEN GAS DETERMINATIONS

Radcalc can calculate the radiolytic production of hydrogen gas in packages containing radioactive material and hydrogenous material, or alternatively, calculate the $G_{effective}$ value for a specified hydrogen gas generation rate. Radcalc calculates percent hydrogen in a specified period of time or will iterate the time needed to reach a specified hydrogen gas concentration. Radcalc also calculates pressure buildup due to hydrogen accumulation. Radcalc 4.0 uses a condensed version of the G value database documented in WHC-SD-TP-RPT-014, *Progress Report for the Enhancement of Radcalc: Isotope Database, Gamma Absorption Fractions, and G(H2) Values*. The basis of G values is documented in DFSNW-RPT-059, *Summary Report of G Value Data for Hydrogen Gas Generation* and DFSNW-ECAL-030 documents the previously established G value database; there have been no changes from the G values used in Radcalc 3.0.1. An updated G value database has been published as DFSNW-ECAL-218, *Radcalc G Value Database*; however, this updated database has not yet been incorporated in the Radcalc software.

3.0 MODIFICATIONS INCORPORATED IN RADCALC 4.0

Radcalc 4.0 is a planned upgrade to Radcalc 3.0.1 initiated through Problem Report/Change Request (PR\CR)-022, *Upgrade from Radcalc 3.0.1 to Radcalc 4.0*. PR/CR-022 identifies 30 items to be revised. Item 1 involves incorporating selected regulatory changes published in 69 FR 3632 (January 26, 2004), "Hazardous Materials Regulations; Compatibility With the Regulations of the International Atomic Energy Agency." These new regulations are anticipated to become effective October 1, 2004. Because Radcalc 4.0 is being released in advance of formal publication of the new regulations, differences, if any, between 69 FR 3632 and DOT regulations published in Title 49 of *Code of Federal Regulations* (CFR) Subchapter C, "Hazardous Materials Regulations," October 1, 2004, edition are not reflected in Radcalc 4.0. It is the user's responsibility to verify that source documents used in development of Radcalc 4.0 are appropriate and current for calculations the user is performing.

PR/CR-022 Item 2 involves adding a new capability to calculate DE-Ci values (see Section 2.4).

Table 3-1 shows changes to Radcalc determination criteria between Radcalc 3.0.1 (now obsolete) and Radcalc 4.0 (executable file dated September 10, 2004).

A number of user- and staff-recommended changes have also been incorporated in Radcalc 4.0. These changes are primarily clarifications to the input or output screens, reference updates, user conveniences, or completeness checks. About half the changes identified in PR/CR-022 are shown in the accompanying figures but the other changes are not easily displayed in this format. In addition, a number of clarifications not specifically identified in PR/CR-022 have also been incorporated.

Table 3-1. Changes from Radcalc 3.0.1 to Radcalc 4.0 Criteria

	Radcalc 3.0.1 (obsolete)	Radcalc 4.0
Radioactive	49 CFR 173.403, 173.433, 173.435, 173.436	Revised A_1 and A_2 values* Activity concentration for exempt material* Activity limit for an exempt consignment*
Type A or Type B	49 CFR 173.403, 173.433, 173.435	No change*
Effective A_1 or A_2 for mixture	49 CFR 173.433	No change*
Limited quantity	49 CFR 173.403, 173.425	No change*
Low specific activity	49 CFR 173.403, 173.427	New LSA-I definitions*
Highway route controlled quantity	49 CFR 173.403	No change*
Fissile quantity Fissile excepted	49 CFR 173.403 49 CFR 173.453	Delete ^{238}Pu as a fissile isotope* New exception determination criteria*
Reportable quantity	49 CFR 172.101, Table 2 to Appendix A	No change*
Transuranic	DOE M 435.1-1	DOE M 435.1-1, Chg. 1; no change
Fissile gram equivalent	TRAMPAC, Rev. 18 (Westinghouse 1999)	Rev. 19C (WTS 2003); no change
^{239}Pu-equivalent activity	DOE/WIPP-02-3122, Rev. 0.1	Rev. 1; no change
Category I, II, or III	Regulatory Guide 7.11 (NRC 1991)	No change
^{239}Pu dose-equivalent curie	-	FGR 11/EPA-520/1-88-020; ICRP 71/72

*Radcalc 4.0 regulatory changes are based on 69 FR 3632. The user must verify that there are no differences between 49 CFR, Subchapter C as published in October 2004 and 69 FR 3632.

49 CFR 172, 2000, "Hazardous Materials Table, Special Provisions, Hazardous Materials Communications, Emergency Response Information, and Training Requirements," *Code of Federal Regulations*, U.S. Department of Transportation, Washington, D.C.

49 CFR 173, 2000, "Shippers – General Requirements for Shipments and Packagings," *Code of Federal Regulations*, as amended, U.S. Department of Transportation, Washington, D.C.

69 FR 3632, 2004, "Hazardous Materials Regulations; Compatibility With the Regulations of the International Atomic Energy Agency," *Federal Register*, Vo. 69, No. 16, pp. 3632-3696 (January 26).

DOE/WIPP-02-3122, 2002, *Contact-Handled Transuranic Waste Acceptance Criteria for the Waste Isolation Pilot Plant*, Rev. 0.1, U.S. Department of Energy, Carlsbad, New Mexico.

DOE/WIPP-02-3122, 2004, *Contact-Handled Transuranic Waste Acceptance Criteria for the Waste Isolation Pilot Plant*, Rev. 1, U.S. Department of Energy, Carlsbad, New Mexico.

DOE Manual 435.1, 1999, *Radioactive Waste Management Manual*, U.S. Department of Energy, Washington, D.C.

DOE Manual 435.1-1, Chg. 1, 2001, *Radioactive Waste Management Manual*, U.S. Department of Energy, Washington, D.C.

FGR11/EPA-520/1-88-020, 1988, *Limiting Values of Radionuclide Intake and Air Concentration and Dose Conversion Factors for Inhalation, Submersion, and Ingestion*, Federal Guidance Report No. 11, U.S. Environmental Protection Agency, Washington, D.C.

ICRP 71, 1996, *Age-Dependent Doses to Members of the Public from Intake of Radionuclides: Part 4 Inhalation Dose Coefficients*, ICRP Report No. 71, International Commission on Radiological Protection, New York, New York.

ICRP 72, 1996, International ICRP Report No. 72, *Age-Dependent Doses to Members of the Public from Intake of Radionuclides: Part 5 Compilation of Ingestion and Inhalation Dose Coefficients*, ICRP Report No. 72, Annals of the ICRP, Vol. 25/3, International Conference for Radiological Protection, Vienna, Austria.

NRC, 1991, Regulatory Guide 7.11, *Fracture Toughness Criteria of Base Material for Ferritic Steel Shipping Cask Containment Vessels with a Maximum Wall Thickness of 4 Inches (0.1 m)*, U.S. Nuclear Regulatory Commission, Washington, D.C.

Westinghouse, 1999, *TRUPACT-II Authorized Methods for Payload Control (TRAMPAC)*, Rev. 18, Westinghouse, Carlsbad, New Mexico.

WTS, 2003, *TRUPACT-II Authorized Methods for Payload Control (TRAMPAC)*, Rev. 19C, Washington TRU Solutions, Carlsbad, New Mexico.

DOE   U.S. Department of Energy

Figures 3-1 and 3-2 provide an example of the modified output of Radcalc 4.0 output using an artificial calculation file. **Bold** fields indicate revisions to the output, with ~~strikeouts~~ being deletions. Shaded fields indicate instructions, guidance, formatting or general information regarding the display. A box identifies the associated PR/CR-022 Item number. A number of minor editorial changes to improve the readability of the output are also shaded. Items to be changed, as identified in PR/CR-022 include:

Item 3:   Report the sum of the activities in Becquerels with and without daughters.

Item 4:   Revise low-specific activity (LSA) output to read "A_2/gm" rather than "specific activity."

Item 5:   Update source document references to the most current versions including: (Note: Data referenced in these documents have not changed from the previous versions.)

DOE/WIPP-02-3122, 2004, *Contact-Handled Transuranic Waste Acceptance Criteria for the Waste Isolation Pilot Plant*, Rev. 1, U.S. Department of Energy, Carlsbad, New Mexico.

DOE Order 435.1-1, Chg. 1, 2001, *Radioactive Waste Management Manual*, U.S. Department of Energy, Washington, D.C.

WTS, 2003, *TRUPACT-II Authorized Methods for Payload Control (TRAMPAC)*, Rev. 19C, Washington TRU Solutions, Carlsbad, New Mexico.

Item 6:   Revise selected Help files to reflect software changes within the limits of funding and time.

Item 7:   Revise output to return "NA" in the lines displaying type, limited quantity, LSA I/II/III, highway route controlled quantity, and fissile excepted determinations if a package is not radioactive.

Figure 3-2 shows an abbreviated example output display for a non-radioactive package.

Item 8:   Add a data file export option for the decayed Export Data File containing the following information: isotope, half-life, activity, specific heat, A_2s, Activity Concentration for Exempt Material (ACEM), Activity Limit for Exempt Consignments (ALEC), fissile-gram equivalents, ^{239}Pu equivalent curies, FGR11, and ICRP 71/72 values for the input source.

The data file option will open and write to Microsoft Excel[10]. The user will be required to save the Excel file from that application. Figure 3-3 is an example the anticipated data file content.

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[10] Excel is a registered trademark of the Microsoft Corporation, Redmond, Washington.

Figure 3-1. Radcalc 4.0 Output Display Changes. (4 pages total)

Radcalc **4.0**   Update version number   [Date file run]
File: [Radcalc file name]

                                                          Performed By:
                                                          Checked By:

Align text on output to improve readability
================================= Input Information =======================================

Source ~~from Input~~: Change to **Data:**

Isotope:	Ci:	Bq:	Gm:	
				Remove colons
Sr-90	0.0171	632700000	0.0001232	
Cs-137	0.0207	765900000	0.0002392	
Pu-238	3.29	1.217E+11	0.1921	
Pu-239	12.2	4.514E+11	196.7	
Pu-240	7.2	2.664E+11	31.73	Present source data in sci. notation (4 sig. digits)
Pu-241	281	1.04E+13	2.728	
Pu-242	0.000281	10400000	0.07106	
Am-241	14.6	5.402E+11	4.26	

If Source option, threshold value has been entered add the following:
Radionuclides with an activity of less than [threshold value] will not be shown in the output: Item 28
(Threshold value will be displayed in unit selected by the user).

Container Data: Add heading
    Container Void Volume: 0   [unit]   Apply units identified by user
    Container Mass: **xxxx**   [unit]   Add container mass
    Gamma Abs Curve: DOT Calculations

Waste Data: Add heading
    Waste Form: Normal
    Waste State: **Solid**   Revise input echo to include Liquid Uranyl Nitrate
    Waste Volume: 1   m^3
    Waste Mass: 1 kg
    Mass of beryllium, lead, graphite,
      and hydrogenous
      material enriched with deuterium   xx [unit]   Add new fissile determination input
    Waste True Density: 0   \   Remove "\"; should be "/" in units   Item 9

G Value Materials **Data:**   Modify title, change "Weight" to "Weight Fraction" and delete the redundant "Weight %"

Weight **Fraction**	~~Weight %~~	G Alpha	G Beta	G Gamma	Material Name
0.5	~~0.5~~	1.6	0.53	0.45	Water (liquid)
0.5	~~0.5~~	0	0	0	USER

G Value Data:

G Alpha	G Beta	G Gamma
0.8	0.265	0.225

                          G values calculated from the list of materials (above).

Decay Time Data: Add heading
    Time to decay source before ~~seal time~~: 0 day   Change to **sealing:**
    Time container is sealed: 0 yr

Comments:

Figure 3-1. Radcalc 4.0 Output Display Changes. (4 pages total)

```
============================== Calculated Results ==============================
Decay Heat:
    Heat Generated at Time Zero:      xxxx          W       Add decay heat at time zero              Item 23
    Heat Generated at Seal Time:      1.21          W       Change to When Sealed
    Heat Generated When Opened:       xxxx          W       Add decay heat when opened

Hydrogen Gas:
    H2 Concentration:        83             %
    H2 Moles :               33.98          moles
    H2 Volume :              761700         cm^3      (0 C, 101.325 kPa)
    H2 Rate When Sealed:     16.93          cm^3/hr   (0 C, 101.325 kPa)      Move condition information
    H2 Rate When Opened:     17.79          cm^3/hr   (0 C, 101.325 kPa)

Helium Gas:
    He Concentration:        0.0019         %
    He Moles :               0.0007913      moles
    He Volume :              17.74          cm^3      (0 C, 101.325 kPa)
    He Rate When Sealed:     0.0003944      cm^3/hr   (0 C, 101.325 kPa)      Add helium
    He Rate When Opened:     0.000414       cm^3/hr   (0 C, 101.325 kPa)

Pressure When Opened:
    Partial Pressure (H2):              83.9         kPa
    Partial Pressure (He):              0.001953     kPa            Add helium
    Partial Pressure (O2):              41.95        kPa       (if H20 present in waste)
    Total Pressure (H2 + He + Air):     185.2        kPa
    Total Pressure (H2 + He + O2 + Air): 227.2       kPa       (if H20 present in waste)

Transportation:
Note: Calculations are made at user-specified decay time.

Radioactive Determination:                                     Provide new explanations
    Radioactive:                   Yes (specific activity > 2 nCi/gm)   (ACEMs and ALECs > 1.0)
    ACEM Limit Fraction            xxxx          ACEMs            (Number of ACEMs)
    ALEC Limit Fraction            xxxx          ALECs            (Number of ALECs)
This package is not exempt from the HMR.                        Add provisions

or

This package may be shipped exempt from the HMR provided the sum of the Fractions of Activity Limits for Exempt
Consignment for all packages in the consignment is less than or equal to 1.0. See 49 CFR 173.403.

or

This package may be shipped exempt from the HMR. See 49 CFR 173.403.


        Specific Activity:       318300000 nCi/gm               Move specific activity to LSA Determination
                                 1.178E+10 Bq/gm

Effective A2s for Mixture:            0.0401             Ci

Type Determination:
    Type:                    B       (A2 unity fraction > 1.0)   (A2s > 1.0) Change to
    A2 Unity Limit Fraction: 7934              A2s                (Number of A2s) Modify text      Item 14

Limited Quantity Determination:
    Limited Quantity:        No                (aActivity > 0.001 A2)
    Activity:                7934              A2
                             318.3             Ci
                             11.78             TBq
U-235 Activity:              0.09835           gm
    The user must check to be sure that all other requirements for LQ in 49 CFR 173.421 are met.
```

Figure 3-1. Radcalc 4.0 Output Display Changes. (4 pages total)

LSA Determination:
    LSA-I: No (~~specific activity > 1E-06 A2/gm~~) add new explanations   Item 4
    LSA-II: No (~~specific activity~~ > 0.0001 **A2/gm**) Replace specific activity with **A2/gm**
    LSA-III: No (~~specific activity~~ > 0.002 **A2/gm**)   Replace specific activity with **A2/gm**
    Specific Activity: **7.934**   **A2/gm**   Item 24
                              xxxx   Ci/gm   Move down from Radioactive Determination
    The user must check to be sure that all other requirements for LSA in 49 CFR 173.403 and 49 CFR 173.427 are met.

HRCQ Determination:
    HRCQ: Yes   (A2**s** ~~unity fraction~~ > 3000)
    A2 ~~Unity~~ **Limit** Fraction: 7934   **A2s**
    Activity: 318.3   Ci
                            11.78   TBq

Fissile **Excepted** Determination:
    Fissile Excepted: Yes   (fissile grams per liter <= 0.5)
    Fissile Quantity: 199.6   gm
    Beryllium, lead, graphite, and
      hydrogenous material
      enriched with deuterium   xxxx   gm
    Solid Non-Fissile Quantity: xxxx   gm
    Total Uranium Quantity: xxxx   gm   Add new fissile-excepted criteria
    U-233 Quantity: xxxx   gm
    U-235 Quantity: xxxx   gm
    Uranium Enrichment: xxxx   %
    Total Plutonium Quantity: xxxx   gm
    Pu-239 Quantity: xxxx   gm
    Pu-241 Quantity: xxxx   gm
~~**Fissile Concentration:**~~   ~~**0.1996 gm/liter**~~
    ~~**The user must check to be sure that all other requirements for Fissile Excepted in 49 CFR 173.453 (d) are met.**~~

Container Category Determination: Add title
    Container Category: I

TRU Waste Determination:
    TRU Waste: Yes   (TRU activity > 100 nCi/gm)
    TRU Activity: 37290000   nCi/g

WIPP Quantities:
    FGE Value: 203.7
    PE-Ci Value: 42.5

Reportable Quantity Determination:
    Reportable Quantity: Yes   (RQ**s** ~~unity fraction~~ >= 1.0)
    RQ ~~Unity~~ **Limit** Fraction: 4010   **RQs**   **(Number of RQs)**

Dose-Equivalent Curie Information:
    Total ICRP71/72 DE-Ci: xxxx
    Total FGR11 DE-Ci: xxxx

Figure 3-1. Radcalc 4.0 Output Display Changes. (4 pages total)

Source at the Start of Seal Time:

Isotope:	Ci:	Bq:	Gm:		
Sr-90	0.0171	632700000	0.0001232		
Cs-137	0.0207	765900000	0.0002392		
Pu-238	3.29	1.217E+11	0.1921		
Pu-239	12.2	4.514E+11	196.7	Report in Sci. notation to 4 sig. digits	
Pu-240	7.2	2.664E+11	31.73		
Pu-241	281	1.04E+13	2.728		
Pu-242	0.000281	10400000	0.07106		
Am-241	14.6	5.402E+11	4.26		
	_____	_____			
Total Activity:	318.3 ~~Ci~~	xxxx		Report total Bq	Item 3
w/o Daughters:	318.3 ~~Ci~~	xxxx		Report total Bq without Daughters	

Shipping Papers and Labels: Item 11

	Isotope:	Number of A2s:	Fraction of A2s:	Cumulative A2s:	**Cumulative Fraction of A2s:**	
*	Am-241	2699	0.3402	2699	xxxx	
*	Pu-239	2255	0.2842	4954	xxxx	Add column of values
*	Pu-240	1331	0.1678	6285		
*	Pu-241	1041	0.1312	7325		
*	Pu-238	608.1	0.07665	7934		
	Pu-242	0.05194	6.547E-06	7934		
	Sr-90	0.006333	7.983E-07	7934		
	Cs-137	0.001533	1.933E-07	7934		

* Contains 95% of the total A2s and must be included per 49 CFR 173.433

Radionuclides comprising less than 0.1% of total A2s are not shown in the list.   Item 10

Figure 3-2. Abbreviated Nonradioactive Package Display Example.

```
==================================== Input Information ====================================
Source from Input:
        Isotope:        Ci:             Bq:             Gm:
        Sr-90           4.0E-09         148             2.881E-11
        Y-90            4.0E-09         148             7.357E-15
        Cs-137          1.0E-09         37              1.155E-11
        Ba-137m         9.46E-10        35              1.759E-18

Waste State:            Solid
Waste Volume:           21700 m^3
Waste Mass:             100 kg
============================== Calculated Results ==============================
Radioactive Determination:
        Radioactive:            No              (specific activity <= 70 Bq/gm)
```

**This package may be shipped exempt from the HMR provided the sum of the Fractions of Activity Limits for
Exempt Consignment for all packages in the consignment is less than or equal to 1.0. See 49 CFR 173.403.**
or

This package may be shipped exempt from the HMR. See 49 CFR 173.403.

```
Type Determination:
        Type:                   A̶  (A2 unity fraction <= 1.0)   revise to:  NA (non- radioactive)    | Item 7 |
        A2 Unity Fraction:      1.556E-09                                                             (typical)

Limited Quantity Determination:
        Limited Quantity:       Yes  (activity <= 0.001 A2)      revise to:  NA (non- radioactive)

LSA Determination:
        LSA-I:          Yes     (specific activity <= 1E-06 A2/gm)    revise to: NA (non- radioactive)
        LSA-II:         Yes     (specific activity <= 0.0001 A2/gm)   revise to: NA (non- radioactive)
        LSA-III:        Yes     (specific activity <= 0.002 A2/gm)    revise to: NA (non- radioactive)

HRCQ Determination:
        HRCQ:           No              revise to:  N.A. (non- radioactive)

Shipping Papers and Labels:
        NA              (non- radioactive)          revise to:
        Isotope:        Number of A2s:  Fraction of A2s:  Cumulative A2s:
*       Sr-90           1.481E-09         0.9524          1.481E-09
```

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Figure 3-3. Example Export Data File Format.

File: C:\Program Files\Duratek\Radcalc 4.0\Verify\VnVTest.rad																					
Date: 8/31/2004																					
A threshold value of 0 Ci was applied.																					
The source as input was multiplied by 1																					
Decay Time: 5 yr																					
						Source When Sealed															
Isotope	Half-Life	Activity			Specific Heat		A2		ACEM		ALEC		FGE		PE-Ci		FGR-11		ICRP-71	
	sec	Ci	Bq	Gm	W/Ci	W	Ci	Fraction	Ci/g	Fraction	Ci	Fraction	Factor	FGEs	Factor	PE-Cis	Factor	DE-Ci	Factor	DE-Ci
Hg-206	489	1.07E-21	3.95E-11	9.52E-30	0.003141	3.35E-24	0.54	0	2.7E-10	0	2.7E-07	0	0		0		0		0	

Item 9:   Delete the "\" appearing in the output when a zero (0) value is entered in the Waste True Density field and correct the units to "kg/m3" when a non-zero value is entered in the Waste True Density field.

Item 10:   Report only those isotopes that exceed 0.1% of the total A_2s in the Shipping Papers and Labels output. Notify the user of this limitation.

Item 11:   Show the cumulative fraction of A_2s in the Shipping Paper and Labels output.

Item 12:   Provide a warning that the input cannot be imported when a user attempts to import a source term containing an invalid isotope, value, or unit.

Item 13:   Revise the Comments field to respond without error to nonalphanumeric keys. Advise the user how to insert a hard return.

Item 14:   Change the field name to "Number of A_2s" and add "A_2s" as the unit.

Item 15:   Enable Radcalc 4.0 to open Radcalc 3.0 and 3.0.1 files. Provide a warning that additional data are required to execute a Radcalc 4.0 calculation.

Item 16:   Set Export initial source term default to 4 significant digits. Allow the user to modify the number of significant digits on a file-by-file or default basis. Expand the range of allowable units to include TBq, moles, and atoms.

Item 17:   Expand the acceptable isotopic source term Import formats from that in Radcalc 3.0.1 (e.g., Ba-137m) to recognize other common formats (e.g., Ba137m, 561371).

Item 18:   Allow users to sort isotopes by name in addition to ZAID (nuclide identification number). Allow the user to set the ordering as a default condition and on a file-by-file basis.

Item 19:   Allow users to change the default font so that each new .rad file will open in that font. Allow the user to continue to modify fonts on a file-by-file basis.

Item 20:   Modify Radcalc to recognize that re-inputting the same data is not a change to the input data such that previously calculated values will be preserved.

Item 21:   Allow the user to establish a default number of significant digits and to change the significant digits for each .rad file.

Item 22:   Allow the user the ability to add and edit materials and material properties (G values) in the G Value Calculation Window.

Item 23:   Add Heat Generated on Start Date (0 decay time) to the output.

To avoid confusion the test will read: "Heat Generated at Time Zero".

Item 24:   Report specific activity in one location on the output in units of A_2/gm and Ci/gm.

Item 25:   Add the capability to export Source When Opened.

Item 25 requires the file menu to be revised to include "Source When Opened" under the "File" menu, "Export Source" option.

Note: This option is only available for hydrogen gas calculations.

Item 26:   Add the capability to modify Page Setup and adjust the number of recent file titles that will be viewed.

Item 27:   Add the close window icon to the top-right corner of the Radcalc windows.

Item 28:   Move the source term multiplication and viewing threshold from the Options window to the Source Term window.

Item 29:   Modify the Source Term window such that entering a new isotope in the Isotope Search box automatically switches the user to Show All Isotopes.

Item 30:   Remove the option to enter the time of day in the Date entry boxes in the Decay and Seal Time windows.

The software version will be revised to indicate Radcalc 4.0. The software version will be stored in *.rad files and printed on hardcopy output.

Changes incorporated into Radcalc 4.0 were documented in DTS-SQA-006, Radcalc *Software Requirement Specification* and DTS-SQA-008, *Radcalc Software Design Description and Implementation Document*.

Table 3-2 provides a description of the Radcalc output.

4.0 LIMITATIONS

Users are responsible to be aware of and account for the limitations as described below:

- Users are responsible for understanding, interpreting, and using regulations and guidance documents and the software.

- Use of files created in previous versions of Radcalc may require input of additional data.

- The new regulations 69 *Federal Register* 3632 are anticipated to become effective October 1, 2004. Because Radcalc 4.0 will be released in advance of formal publication of the new regulations, differences, if any, between 69 FR 3632 and DOT regulations published in 49 CFR Subchapter C, "Hazardous Materials Regulations" (October 1, 2004), will not be reflected in Radcalc 4.0.

- It is the user's responsibility to verify that source documents used in development of Radcalc 4.0 are appropriate and current for calculations the user is performing.

- The new DOT regulations report A_1 and A_2 values (in TBq and Ci) to two significant digits. The old regulations reported one significant digit for TBq (consistent with the International Atomic Energy Agency [IAEA] source document), converted to Ci (multiplying by 0.037), and reported three significant digits for the Ci values, which resulted in a perception that the Ci value was more accurate. In fact the three significant digits were not justified (only one significant digit was justified). The new DOT regulations "report" two significant digits for TBq by adding an extraneous 0 onto the one significant digit value in the IAEA source document. The Ci values are again obtained by multiplying by 0.037 resulting in a Ci value reported to two significant digits (again only one is really justified). However, some DOT Ci values are rounded down (e.g., Th-231 rounds from 0.541 to 0.54) and some are rounded up (e.g., Th-229 rounds from 0.0135 to 0.14). Use of DOT Ci values that are rounded down will produce a slightly conservative number of A_1s or A_2s relative to using TBq values; use of DOT Ci values that are rounded up will produce slightly non-conservative numbers relative to using TBq values.

- Radcalc calculations are performed with double precision (i.e., calculations carried to a minimum of 1E308). Some discrepancies may occur between double precision calculations and hand calculations using fewer significant figures, particularly in cases where there are large variations in the magnitude of the input values.

- Radcalc performs calculations based on the input values for a single package. 69 FR 3632 (e.g., 49 CFR 173. 436, "Exempt material activity concentrations and exempt consignment activity limits for radionuclides") requires calculation of consignment limits. Radcalc 4.0 does calculate the activity limit for exempt consignments; however, because Radcalc input is limited to a single package, the activity limit for exempt consignment is valid only on a package-by-package basis (i.e., there is only one package in the consignment). The user must make multi-package consignment determinations separately.

Table 3-2. Description of Radcalc 4.0 Output (4 pages total)

Output Parameter	Units	Description
Decay Heat:		
Heat Generated at Time Zero:	W	Rate of heat generation at time zero.
Heat Generated at Seal Time:	W	Rate of heat generation at seal time.
Heat Generated at Opening:	W	Rate of heat generation at time of opening.

Hydrogen Gas: (0 C, 101.325 kPa; ideal gas) – displayed for hydrogen gas calculations only

H2 Percent Concentration:	%	Mole percent hydrogen in the total void volume of container.
H2 Moles:	moles	Moles of hydrogen.
H2 Volume:	cm^3	The volume of the hydrogen.
H2 Rate When Sealed:	cm^3/h	Hydrogen generation rate at seal date.
H2 Rate When Opened:	cm^3/h	Hydrogen generation rate at opening date.

Helium Gas: (0 C, 101.325 kPa; ideal gas) – displayed for hydrogen gas calculations only

He Percent Concentration:	%	Mole percent helium in the total void volume of container.
He Moles:	moles	Moles of helium.
He Volume:	cm^3	The volume of the helium.
He Rate When Sealed:	cm^3/h	Helium generation rate at seal date.
He Rate When Opened:	cm^3/h	Helium generation rate at opening date.

Pressure: (0 C, 101.325 kPa; ideal gas) – displayed for hydrogen gas calculations only

Partial Pressure (H2):	kPa	Partial pressure of the hydrogen in the total void volume.
Partial Pressure (He):	kPa	Partial pressure of the helium in the total void volume.
Partial Pressure (02):	kPa	If substantial water is present, partial pressure of oxygen in the total void volume. Oxygen is assumed to be half of the hydrogen.
Total Pressure (H2+He+Air):	kPa	Total pressure of hydrogen, helium, and air.
Total Pressure (H2+02+He+Air):	kPa	If substantial water is present, total pressure of hydrogen, oxygen, helium, and air. Oxygen is assumed to be half of the hydrogen.

TRANSPORTATION: (Note: Transportation classifications are made at user-specified decay time.)

Radioactive Determination:		
Radioactive:	Yes or No	Yes indicates waste is radioactive as specified in 49 CFR 173.403.
ACEM Limit Fraction	ACEM	Number of ACEMs as listed in 49 CFR 173.436.
ALEC Limit Fraction	ALEC	Number of ALECs as listed in 49 CFR 173.436.
Effective A2s for Mixture:	Ci	The effective A_2 is calculated as outlined in 49 CFR 173.433.
Type Determination:		
Type:	A or B	Radioactive material classification per 49 CFR 173.403.
A2 Limit Fraction:	A_2s	Used for type determination; a value greater than 1 is Type B.

Limited Quantity Determination: (The user must ensure that all 49 CFR 173.421 requirements are met.)

Limited Quantity:	Yes or No	As defined in 49 CFR 173.403.
Activity:	A_2, Ci, TBq	Used for limited quantity determination.
U-235 Activity:	gm	Used for limited quantity determination.

Table 3-2. Description of Radcalc 4.0 Output (4 pages total)

Output Parameter	Units	Description
LSA Determination: (The user must ensure that all 49 CFR 173.403 and 49 CFR 173.427 requirements are met.)		
LSA-I:	Yes or No	LSA-I determination per 49 CFR 173.403.
LSA-II:	Yes or No	LSA-II determination per 49 CFR 173.403.
LSA-III:	Yes or No	LSA-III determination per 49 CFR 173.403.
Specific Activity:	A_2/gm Ci/gm	Used for LSA-I, -II or -III determinations.
HRCQ Determination:		
HRCQ:	Yes, No, NA	Highway route control quantity per 49 CFR 173.403.
A2 Limit Fraction:	A_2s	Used for HRCQ determination.
Activity:	Ci, TBq	Used for HRCQ determination.
Fissile Excepted Determination: (The user must ensure all 49 CFR 173.453 requirements are met.)		
Fissile Excepted:	Yes or No	Fissile-excepted determination per 49 CFR 173.453.
Fissile Quantity:	gm	Mass of Pu-239, Pu-241, U-233, and U-235 per 49 CFR 173.403.
Beryllium, lead, graphite, and hydrogenous material enriched with deuterium:	gm	Used for fissile excepted determination.
Solid Non-Fissile Quantity:	gm	Used for fissile excepted determination.
Total Uranium Quantity:	gm	Used for fissile excepted determination.
U-233 Quantity:	gm	Used for fissile excepted determination.
U-235 Quantity:	gm	Used for fissile excepted determination.
Uranium Enrichment:	%	Used for fissile excepted determination.
Total Plutonium Quantity:	gm	Used for fissile excepted determination.
Pu-239 Quantity:	gm	Used for fissile excepted determination.
Pu-241 Quantity:	gm	Used for fissile excepted determination.
Container Category Determination:		
Container Category:	I, II, or III	Container category determination per NRC Regulatory Guide 7.11.
TRU Waste Determination:		
TRU Waste:	Yes or No	Transuranic determination per DOE Manual 435.1-1, Chg. 1.
TRU Activity	nCi/gm	Used for transuranic waste determination.
WIPP Quantities:		
FGE Value:	gm	Pu-239 fissile-gram equivalents per the TRAMPAC (WTS 2003).
PE-Ci Value	PE-Ci	Pu-239 equivalent curies per DOE/WIPP-02-3122.
Reportable Quantity Determination:		
Reportable Quantity:	Yes or No	Reportable quantity per 49 CFR 172.101 Appendix A.
RQ Limit Fraction:	RQs	Number of RQs. Used for reportable quantity determination.
Dose-Equivalent Curie Information:		
Total ICRP71/72 DE-Ci	DE-Ci	Pu-239 DE-Ci per ICRP 71 and ICRP 72.
Total FGR11 DE-Ci	DE-Ci	Pu-239 DE-Ci per FGR11/EPA-520/1-88-020.

Table 3-2. Description of Radcalc 4.0 Output (4 pages total)

Output Parameter	Units	Description
Source at the Start of Seal Time:		
Isotope List:	Ci, Bq, gm	List of isotopes decayed to user specified decay time with activities above the user-specified output display threshold.
Total Activity	Ci, Bq	Total activity at the end of the user-specified decay time including isotopes below the user-specified output threshold.
Total Activity w/o Daughters	Ci, Bq	Total activity at the end of the user-specified decay time including isotopes below the user-specified output display threshold, but excluding those isotopes designated as "daughters" for transportation classification calculations.
Shipping Papers and Labels:		
Isotope List:	Number of A_1/A_2s Fraction of A_1/A_2s Cumulative number of A_1/A_2s Cumulative fraction of A_1/A_2s	Lists isotopes sorted from highest to lowest number of A_1s or A_2s. An asterisk is placed next to the nuclides that comprise 95% of the total number of A_1s or A_2s for the entire inventory. The nuclides identified with an asterisk must be included on shipping papers and labels per 49 CFR 173.433. Radionuclides comprising less than 0.1% of the total A2s are not shown in the list.

Table 3-2. Description of Radcalc 4.0 Output (4 pages total)

Output Parameter	Units	Description

NOTE: U.S. Department of Transportation regulations are projected based on 69 FR 3632.

49 CFR Subchapter C, October 1, 2004, "Hazardous Materials Regulations," *Code of Federal Regulations*, Research and Special Programs Administration, U.S. Department of Transportation, Washington, D. C.

    172.101, "List of Hazardous Substances and Reportable Quantities, Appendix A" and "Table 2 to Appendix A – Radionuclides."

    173.403, "Definitions."

    173.427, "Transport requirements for low specific activity (LSA) Class 7 (radioactive) materials and surface contaminated objects (SCO)."

    173.433, "Requirements for determining basic radionuclide values, and for the listing of radionuclides on shipping papers and labels."

    173.435, "Table of A_1 and A_2 values for radionuclides."

    173.436, "Exempt material activity concentrations and exempt consignment activity limits for radionuclides."

69 FR 3632, 2004, "Hazardous Materials Regulations; Compatibility With the Regulations of the International Atomic Energy Agency," *Federal Register*, Vol. 69, No. 16, pp. 3632-3696 (January 26), U.S. Department of Transportation, Washington, D.C.

DOE Manual 435.1-1 Chg 1, 2001, *Radioactive Waste Management Manual*, U.S. Department of Energy, Washington, D.C.

DOE/WIPP-02-3122, 2004, *Contact-Handled Transuranic Waste Acceptance Criteria for the Waste Isolation Pilot Plant*, Rev. 1, U.S. Department of Energy, Carlsbad, New Mexico.

FGR11/EPA-520/1-88-020, 1988, *Limiting Values of Radionuclide Intake and Air Concentration and Dose Conversion Factors for Inhalation, Submersion, and Ingestion*, Federal Guidance Report No. 11, U.S. Environmental Protection Agency, Washington, D.C.

ICRP Report No. 71, 1996, *Age-Dependent Doses to Members of the Public from Intake of Radionuclides: Part 4 Inhalation Dose Coefficients,* International Commission on Radiological Protection, New York, New York.

ICRP Publication 72, 1996, *Age-Dependent Doses to Members of the Public from Intake of Radionuclides: Part 5 Compilation of Ingestion and Inhalation Dose Coefficients*, Annals of the ICRP, Vol. 25/3, International Conference for Radiological Protection, Vienna, Austria.

Regulatory Guide 7.11, 1991, *Fracture Toughness Criteria of Base Material for Ferritic Steel Shipping Cask Containment Vessels with a Maximum Wall Thickness of 4 Inches (0.1 m)*, U.S. Nuclear Regulatory Commission, Washington, D.C.

WTS, 2003, *TRUPACT-II Authorized Methods for Payload Control (TRAMPAC)*, Rev. 19C, Washington TRU Solutions, Carlsbad, New Mexico.

ACEM	activity concentration for exempt materials	LSA	low-specific activity
ALEC	activity limit for exempt consignments	NRC	U.S. Nuclear Regulatory Commission
DE-Ci	Pu-239 dose-equivalent curie	PE-Ci	Pu-239 equivalent curie
DOT	U.S. Department of Transportation	RQ	reportable quantity
FGE	Pu-239 fissile-gram equivalent	TRU	transuranic
HRCQ	highway route controlled quantity	WIPP	Waste Isolation Pilot Plant
LQ	limited quantity		

- For LSA-I, II, III calculations the user must check 49 CFR 173.403 and 49 CFR 173.427 to verify that <u>all</u> requirements for LSA are met. Radcalc does not check all LSA requirements.

- Radcalc does not evaluate all criteria, especially those that are qualitative in nature (e.g., the origin of the material). The user must understand and interpret both numeric and non-numeric requirements established in the regulations, including those Radcalc evaluates.

- 69 FR 3632 (49 CFR 173.403) has removed ^{238}Pu from the definition of "fissile material." DOE/WIPP-02-3122 does include ^{238}Pu in the calculation of FGE. Therefore, if a large quantity of ^{238}Pu is present in a package, the package contents may not be considered fissile material as define in DOT regulations even though there is a large number of FGEs.

- Radcalc evaluates fissile-excepted status in accordance with numeric criteria in 49 CFR 173.453(a) and (f) but does not check nonnumeric fissile-excepted criteria. The user must perform these checks separately.

- Transportation classification is calculated for the end of the decay time, which may be 0.

- Pressure is calculated at the end of the seal time or at the open date, depending on whether time mode or date mode has been selected in the time window.

- Sum of activity after seal time includes all isotopes (isotope threshold value ignored).

- The effective A_2s for the mixture allows one to calculate total A_2s using the formula: Total Activity in Package/A_2s for mixture = Total A2s. If a large quantity of a consistent waste steam is produced, one could measure or calculate the activity in each package, then divide it by the A_2s for mixture value to quickly calculate A_2s.

- Only personnel familiar with the terminology, methodologies, and limitations of hydrogen gas calculations should use Radcalc hydrogen gas calculation capabilities.

- Hydrogen gas calculations are limited to radiolytic production of hydrogen gas. Radcalc does not account for hydrogen gas generated due to corrosion, chemical decomposition, or biological activity. Radcalc cannot be used to calculate hydrogen gas generation for spent nuclear fuel applications, which requires case-specific analysis.

- Radcalc hydrogen gas calculations do not account for matrix depletion and recombination.

- G values are material- and decay-type specific; however, the $G_{effective}$ value calculated in Radcalc is averaged for all decay types present.

- Radcalc calculates the total decays of each isotope for H_2 gas generation calculations. The helium calculation takes the total decays value for each isotope, searches the database for an alpha decay branching ratio, and if it finds one it multiplies the total decays by the branching ratio to give the helium production in atoms for each isotope. The calculation sums the

contributions by isotope to find the total helium atoms produced. Then it uses the same unit conversion routines as the hydrogen gas calculation to give pressure and volume.

- Some users may desire or prefer DE-Ci values defined in DOE-EH-0071, *Internal Dose Conversion Factors for Calculation of Dose to the Public* (1988) as a formal U.S. Department of Energy (DOE) publication, or ICRP CD-1, *Database of Dose Coefficients: Workers and Members of the Public*, which is the most up-to-date source available and includes dose coefficients for workers previously published in ICRP 68, *Dose Coefficients for Intakes of Radionuclides by Workers*. The user must understand the purpose and limits of the reference material selected.

- Not all Help files have been updated due to time and funding constraints. If required, the user should review the support documentation and/or contact the developers for clarification.

- The .iso files used with the DE-Calc software at the Hanford Site uses decayed source term and defaults to initial source for 0 decay time.

Additional general information and limitations are provided in the Radcalc manuals.

5.0 QUALITY ASSURANCE

Duratek Technical Services (DTS) has developed and maintains Radcalc on behalf of the DOE National Transportation Program. DTS work is performed under a DOE-approved quality assurance (QA) Program documented in DTS-QAM-001, *Duratek Technical Services Quality Assurance Manual*, which is based on the following.

- 18 Basic Requirements prescribed in 10 CFR 71, "Packaging and Transportation of Radioactive Materials," Subpart H, "Quality Assurance."

- 10 CFR 72, "Licensing Requirements for the Independent Storage of Spent Nuclear Fuel, High-Level Radioactive Waste, and Reactor-Related Greater than Class C Waste," Subpart G "Quality Assurance."

- 10 Criterion prescribed in 10 CFR 830, "Nuclear Safety Management" and 830.122, "Quality assurance criteria."

- DOE Order 414.1, *Quality Assurance*.

- 18 Basic and Supplement Requirements of American Society of Mechanical Engineers (ASME) NQA-1-1994, *Quality Assurance Requirements for Nuclear Facility Applications*.

Implementation of the DTS QA Program described in DTS-QAM-001 is accomplished through written, approved procedures documented in DTS-QAP-001, *Duratek Technical Services Quality Assurance Procedures*, Quality Procedure (QP) 3-10, "Software Management." Radcalc is a Level-1 software (software used in safety class or safety-significant applications) as defined in QP 3-10.

The *Software Quality Plan* (8/24/04) (DTS 2004), DTS-SQA-006, *Radcalc Software Requirement Specification*, and DTS-SQA-008, *Radcalc Software Design Description and Implementation Document* document the QA requirements and technical changes to be incorporated in Radcalc 4.0. DTS-VV-021, *Radcalc 4.0 Verification and Validation Test Plan* documents the process by which the QA requirements established in QP 3-10 have been implemented. DTS-VV-022, *Radcalc 4.0 Verification and Validation Test Procedure* documents the step-by-step procedure used to demonstrate the following.

- Compliance with the requirements established in DTS-SQA-006 and DTS-SQA-008
- Successful performance of test cases stipulated in DTS-VV-022, including

  - Adequately and completely performs all intended function
  - Produces correct results for each parameter employed (less than 10% variance)
  - Is valid over the permissible range of operation for the controlled function
  - Properly handles abnormal conditions and events as well as credible failures
  - Does not perform adverse unintended functions
  - Does not degrade the system either by itself, or in combination with other functions.

DTS-VV-023, *Radcalc 4.0 Verification and Validation Test Report* documents that the software has been fully verified and validated in accordance with DTS's DOE-approved QA program.

Radcalc's regulatory, nuclear, atomic mass, DE-Ci, and G value databases were documented and validated separately in accordance with DTS-QAM-001.

Radcalc also includes a user-activated regression test to validate the installation of the software. This validation file may be viewed and printed by navigating to the C:/Program Files/Duratek/Radcalc 4.0/Verify folder and opening the VnVTest.rad file.

6.0 USER SUPPORT

Radcalc is available free to users as a service of the DOE National Transportation Program. The software can be downloaded from http://www.doe-radcalc.com. Software documentation is available to registered users.

Documentation is available in four volumes including:

- DFSNW-RPT-065, *Radcalc Volume I: User's Manual* (intended to familiarize the user with the software)

- DFSNW-RPT-042, *Radcalc 3.0 Volume II: Technical Manual* (theoretical background, calculation methodology, configuration control, and historical information);

- DTS-SQA-009.3, *Radcalc Volume III: Quality Assurance Report*

- DFSNW-RPT-042, *Radcalc 3.0 Volume IV: Database Manual*.

Due to funding limitations only Volume III has been updated in time for the September 2004 release of the software. Additional volumes will be released as funding allows. Registered users may download the manuals from the download page.

Radcalc is distributed with a database viewer that allows users to access the Radcalc nuclear, transportation classification, and G value database values on an isotope-by-isotope basis.

User-funded training in the use of Radcalc's transportation and hydrogen gas modules is offered periodically when sufficient students express interest. Training may be provided at facilities in Richland, Washington, or may be arranged at sites convenient to the user.

A list containing known issues with Radcalc and user-requested changes will be maintained on the Radcalc website. User input is encouraged.

Questions may be directed by E-mail or phone to the following individual.

    Larry Stuhl   (509) 375-9530

EnergySolutions, Federal Services, Inc.
2345 Stevens Drive, Suite 240
Richland, Washington 99354

7.0 REFERENCES

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